Lecture 3

Introduction to optimality conditions

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Overview

Introduction

Existence of optimal solutions

Optimality conditions Unconstrained case Convex feasible set Overview Introduction

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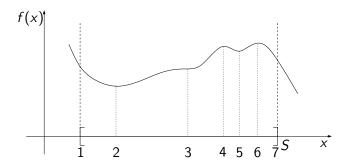
Existence of optimal solutions

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minimize
$$f(\mathbf{x})$$
, (1a)

subject to
$$\mathbf{x} \in \mathcal{S}$$
, (1b)

 $S\subseteq \mathbb{R}^n$ nonempty set, $f:\mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ a given function



- (i) **boundary points** of *S*
- (ii) **stationary points**, that is, where f'(x) = 0
- (iii) discontinuities in f or f'

Here:

- (i) 1, 7
- (ii) 2, 3, 4, 5, 6
- (iii) none

- ► There must exist an optimal solution, **Existence condition**
- ▶ No other point than 1–7 can be optimal **Necessary condition**
- ► Thus, one of the points 1–7 is optimal. By direct computation, it must be 2
 Sufficient condition

▶ $\mathbf{x}^* \in S$ is a **global minimum** of f over S if it attains the lowest value of f over S:

$$f(\mathbf{x}^*) \leq f(\mathbf{x}), \quad \mathbf{x} \in S$$

▶ $\mathbf{x}^* \in S$ is a **local minimum** of f over S if there exists a small enough ball intersected with S around \mathbf{x}^* such that it is an optimal solution in that smaller set: with $B_{\varepsilon}(\mathbf{x}^*) := \{ \mathbf{y} \in \mathbb{R}^n \mid \|\mathbf{y} - \mathbf{x}^*\| < \varepsilon \}$ being the Euclidean ball with radius ε centered at \mathbf{x}^* , we get

$$\exists \varepsilon > 0$$
 such that $f(\mathbf{x}^*) \leq f(\mathbf{x}), \qquad \mathbf{x} \in S \cap B_{\varepsilon}(\mathbf{x}^*)$

▶ $\mathbf{x}^* \in S$ is a **strict local minimum** of f over S if $f(\mathbf{x}^*) < f(\mathbf{x})$ holds above for $\mathbf{x} \neq \mathbf{x}^*$

Overview **Existence**

Introduction

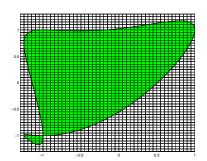
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- ▶ We call S open if for every $\mathbf{x} \in S$ there is an $\varepsilon > 0$ such that $\{z \in \mathbb{R}^n \mid ||z x|| < \varepsilon\} = B_{\varepsilon}(\mathbf{x}) \subset S$. Ex: the interval $(0, \infty)$
- ▶ We call S closed if $\mathbb{R}^n \setminus S$ is open. Ex: the interval $[0, \infty)$.
- ▶ A **limit point** of a set S is a point \mathbf{x} such that there is a sequence $\{\mathbf{x}_k\}_{k=1}^{\infty} \subset S$ where $\mathbf{x}_k \to \mathbf{x}$.
- Can equivalently define a closed as a set which contains all its limit points.
- ▶ If *S* is both closed and bounded it is called **compact**.

Proposition: (Convergent subsequences) Let S be compact and $\{\mathbf{x}_k\}_{k=1}^{\infty} \subset S$. Then there is a **convergent subsequence** $\{\mathbf{x}_{k_i}\}_{i=1}^{\infty}$ where $\lim_{i\to\infty}\mathbf{x}_{k_i}=\mathbf{x}$ for some $\mathbf{x}\in S$.

Intuition:



- ► A sequence is an infinite set of points in *S*
- ▶ Divide *S* into small blocks.
- At least one box contains infinitely many points in the sequence.

Weierstrass' Theorem (simple version): Consider the problem (1), where S is a nonempty, closed and bounded set and f is continuous on S. Then, there exists a nonempty, closed and bounded (i.e., compact) set of optimal solutions to the problem (1)

- Construct a problem such that no optimal solution exists.
- How does it violate Weierstrass theorem?
- 2 min.

 $S \subseteq \mathbb{R}^n$ nonempty and closed, $f: S \to \mathbb{R}$

► *f* is **weakly coercive** with respect to the set *S* if either *S* is bounded or

$$\lim_{\substack{\|\mathbf{x}\|\to\infty\\\mathbf{x}\in S}} f(\mathbf{x}) = \infty$$

holds

▶ The weak coercivity of $f: S \to \mathbb{R}$ is equivalent to the property that f has bounded level sets (Why?)

 $S \subseteq \mathbb{R}^n$ nonempty and closed, $f: S \to \mathbb{R}$

▶ f is lower semi-continuous at $\bar{\mathbf{x}} \in S$ if the value $f(\bar{\mathbf{x}})$ is less than or equal to every limit of f as $\mathbf{x}_k \to \bar{\mathbf{x}}$ In other words, f is lower semi-continuous at $\bar{\mathbf{x}} \in S$ if

$$\mathbf{x}_k \to \bar{\mathbf{x}} \qquad \Longrightarrow \qquad f(\bar{\mathbf{x}}) \leq \liminf_{k \to \infty} f(\mathbf{x}_k)$$

- Lower semi-continuity of f is equivalent to the closedness of all its sub-level sets $\operatorname{lev}_f(b) = \{\mathbf{x} \in S \mid f(\mathbf{x}) \leq b\}, \ b \in \mathbb{R}$, as well as the closedness of its epigraph $\{(\mathbf{x},y): \mathbf{x} \in S, y \geq f(\mathbf{x})\}$ (Why?)
- ► Lower semi-continuous functions in one variable have the appearance shown in the figure on the next slide.
- ▶ Continuity \Leftrightarrow f and -f lower semi-continuous.

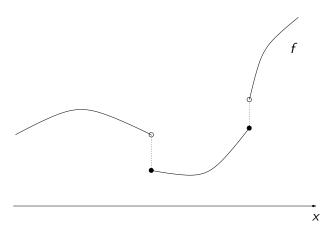


Figure: A lower semi-continuous function in one variable

Weierstrass' Theorem: Let $S \subseteq \mathbb{R}^n$ be a nonempty and closed set, and $f: S \to \mathbb{R}$ be a lower semi-continuous function on S. If f is weakly coercive with respect to S, then there exists a nonempty, closed and bounded (thus compact) set of optimal solutions to the problem (1)

Proof. Let $\bar{\mathbf{x}} \in S$ be any feasible solution. The level set $\bar{S} = \{\mathbf{x} \in S \mid f(\mathbf{x}) \leq f(\bar{\mathbf{x}})\}$ is closed (by lower semi-continuity) and bounded (by weak coercivity). Clearly the optimal solutions of (1) and $\min_{\mathbf{x} \in \bar{S}} f(\mathbf{x})$ coincide. The theorem follows in the same way as the simple version.

Example: $f(\mathbf{x}) = \|\mathbf{x} - \mathbf{y}\|$, S any closed non-empty set, any $\mathbf{y} \in \mathbb{R}^n$. Weierstrass Theorem yields that for any point $\mathbf{y} \in \mathbb{R}^n$, there is always (at least) one 'nearest' point in S.

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Optimality conditions Unconstrained case Convex feasible set Consider the problem (1), where S is a convex set and f is convex on S. Then, every local minimum of f over S is also a global minimum

Proof.

Intuitive image: If \mathbf{x}^* is a local minimum, then f cannot go down-hill from \mathbf{x}^* in any direction, but if $\bar{\mathbf{x}}$ has a lower value, then f has to go down-hill sooner or later. This cannot be the shape of any convex function.

We call $f: \mathbb{R}^n \to \mathbb{R}$ differentiable at \mathbf{x}_0 , if there is a $\nabla f(\mathbf{x}_0)$ such that

$$f'(\mathbf{x}_0; \mathbf{d}) = \lim_{t \to 0} \frac{f(\mathbf{x}_0 + t\mathbf{d}) - f(\mathbf{x}_0)}{t} = \nabla f(\mathbf{x}_0)^{\mathrm{T}} \mathbf{d}$$

for all \mathbf{d} , and call f differentiable if this holds for all \mathbf{x}_0 . If f is differentiable at \mathbf{x}_0 , Taylor's Theorem guarantees the existence of a 'function' o(t) such that

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^{\mathrm{T}}(\mathbf{x} - \mathbf{x}_0) + o(\|\mathbf{x} - \mathbf{x}_0\|),$$

$$\lim_{t \to 0^+} \frac{o(t)}{t} = 0.$$

If $\nabla f(\mathbf{x})$ is continous, then f is called continuously differentiable, denoted by $f \in C^1$. Similarly defined is $f \in C^2$, where we also have

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^{\mathrm{T}} (\mathbf{x} - \mathbf{x}_0) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_0)^{\mathrm{T}} \nabla^2 f(\mathbf{x}_0) (\mathbf{x} - \mathbf{x}_0) + o(\|\mathbf{x} - \mathbf{x}_0\|^2),$$

where the matrix $\nabla^2 f(\mathbf{x}_0) \in \mathbb{R}^{n \times n}$ is called the **Hessian** of f at \mathbf{x}_0 .

If
$$\mathbf{x}^*$$
 is a local minimum of fon \mathbb{R}^n and $f \in C^1$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$

Proof.

Note: the other direction is not true, this is a **necessary** condition (consider $f(x) = x^3$).

Descent direction: Let $\mathbf{x} \in \mathbb{R}^n$. We call \mathbf{p} a direction of **descent** with respect to f at \mathbf{x} if

 $\exists \delta > 0$ such that $f(\mathbf{x} + \alpha \mathbf{p}) < f(\mathbf{x})$ for every $\alpha \in (0, \delta]$

Suppose that $f: \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is in C^1 around a point \mathbf{x} for which $f(\mathbf{x}) < +\infty$, and that $\mathbf{p} \in \mathbb{R}^n$. If $\nabla f(\mathbf{x})^\mathrm{T} \mathbf{p} < 0$ then the vector \mathbf{p} defines a direction of descent with respect to f at \mathbf{x} .

$$\mathbf{x}^*$$
 is a local min of fon $\mathbb{R}^n \implies \begin{cases} \nabla f(\mathbf{x}^*) = \mathbf{0}^n; \\ \nabla^2 f(\mathbf{x}^*) \text{ is p.s.d.} \end{cases}$

Proof.

$$\left. egin{aligned}
abla f(\mathbf{x}^*) &= \mathbf{0}^n \\
abla^2 f(\mathbf{x}^*) & \text{is p.d.} \end{aligned}
ight\} \Longrightarrow \mathbf{x}^* \ \ \text{is a strict local min of f on } \mathbb{R}^n$$

- ▶ Note: n = 1: $x^* \in \mathbb{R}$ is a local minimum $\Longrightarrow f'(x^*) = 0$ and $f''(x^*) \ge 0$
- Note: n = 1: $f'(x^*) = 0$ and $f''(x^*) > 0 \Longrightarrow x^* \in \mathbb{R}$ is a strict local minimum

Let
$$f \in C^1$$
, and f be convex. Then,

$$\mathbf{x}^*$$
 is a global minimum of f on $\mathbb{R}^n \iff \nabla f(\mathbf{x}^*) = \mathbf{0}^n$

Necessary opt. conditions, I: Variational Inequality (VI) Optimality

Suppose $S \subseteq \mathbb{R}^n$, $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is in C^1 around $\mathbf{x} \in S$

- (a) If $\mathbf{x}^* \in S$ is a local minimum of f on S then $\nabla f(\mathbf{x}^*)^{\mathrm{T}}\mathbf{p} \geq 0$ holds for every feasible direction \mathbf{p} at \mathbf{x}^*
- (b) Suppose that S is convex and that f is in C^1 on S. If $\mathbf{x}^* \in S$ is a local minimum of f on S then

$$\nabla f(\mathbf{x}^*)^{\mathrm{T}}(\mathbf{x} - \mathbf{x}^*) \ge 0, \qquad \mathbf{x} \in S$$
 (2)

- ► We refer to (2) as a variational inequality and x* as stationary
- ▶ Suppose $S \subseteq \mathbb{R}^n$ is nonempty and convex. Let $f \in C^1$ on S, convex. Then,

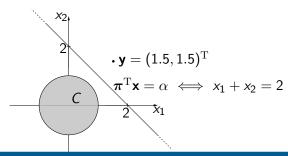
 \mathbf{x}^* is a global minimum of f on $S \iff (2)$ holds

Proof.

▶ Compare with the case $S = \mathbb{R}^n$!

The Separation Theorem was earlier stated and used in order to establish Farkas' Lemma. The VI stationarity conditions, and Weierstrass' Theorem, can be used to establish it.

Suppose that $C\subseteq\mathbb{R}^n$ is closed and convex, and that the point \mathbf{y} does not lie in C. Then there exist a vector $\mathbf{\pi}\neq\mathbf{0}^n$ and $\alpha\in\mathbb{R}$ such that $\mathbf{\pi}^{\mathrm{T}}\mathbf{y}>\alpha$ and $\mathbf{\pi}^{\mathrm{T}}\mathbf{x}\leq\alpha$ for all $\mathbf{x}\in C$



Proof. Consider the problem of finding the closest point to y in C, that is,

$$\min_{\mathbf{x} \in S} h(\mathbf{x})$$

where
$$h(\mathbf{x}) = \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|^2$$

- ▶ Weierstrass guarantees an optimal solution $\mathbf{x}^* \in C$.
- ▶ $(VI) \Rightarrow \nabla h(\mathbf{x}^*)(\mathbf{x} \mathbf{x}^*) \geq 0$ for all $x \in C$.
- $\triangleright \nabla h(\mathbf{x}) = \mathbf{x} \mathbf{y}$
- ▶ Set $\pi := \mathbf{y} \mathbf{x}^* = -\nabla h(\mathbf{x}^*)$ and $\alpha := \boldsymbol{\pi}^{\mathrm{T}}\mathbf{x}^*$
- $\mathbf{y} \notin C \colon \boldsymbol{\pi}^{\mathrm{T}} \mathbf{y} \alpha = (\mathbf{y} \mathbf{x}^*)^{\mathrm{T}} \mathbf{y} (\mathbf{y} \mathbf{x}^*)^{\mathrm{T}} \mathbf{x}^* = \|\mathbf{y} \mathbf{x}^*\|^2 > 0$
- ▶ For any $\mathbf{x} \in \mathcal{C}$, the (VI) yields, $-\boldsymbol{\pi}^{\mathrm{T}}(\mathbf{x} \mathbf{x}^*) \geq 0 \iff \boldsymbol{\pi}^{\mathrm{T}}\mathbf{x} \leq \alpha$
- ▶ The hyperplane provided by the theorem is actually a tangent to C, while the normal is $\mathbf{y} \mathbf{x}^*$

- ▶ In the previous slide we used the solution to the problem $\min_{\mathbf{x} \in S} \|\mathbf{x} \mathbf{y}\|^2$.
- As the objective function $\|\mathbf{x} \mathbf{y}\|^2$ is strictly convex, the solution \mathbf{x}^* is actually a unique solution.
- ▶ So for any $\mathbf{y} \in \mathbb{R}^n$, and a closed convex set S, there is always a **unique** nearest point $\mathbf{x}^* \in S$ to \mathbf{y} .
- We call this point the projection of y onto S. We denote this by Proj_S(y).
- ▶ Characterization from (VI): $\operatorname{Proj}_{S}(\mathbf{y})$ is the (unique) vector such that

$$(\mathbf{y} - \operatorname{Proj}_{S}(\mathbf{y}))^{\mathrm{T}}(\mathbf{x} - \operatorname{Proj}_{S}(\mathbf{y})) \leq 0, \quad \forall \mathbf{x} \in S$$

 $\mathbf{x}^* \in S$ is stationary iff

$$\underset{\mathbf{x} \in \mathcal{S}}{\operatorname{minimum}} \ \nabla f(\mathbf{x}^*)^{\mathrm{T}}(\mathbf{x} - \mathbf{x}^*) = 0$$

- ▶ Proof.
- Method basis: given $\mathbf{x}_k \in S$, find out if we are stationary by minimizing $\nabla f(\mathbf{x}_k)^{\mathrm{T}}(\mathbf{x} \mathbf{x}_k)$ over $\mathbf{x} \in S$. In some sense, we find the $\mathbf{x} \in S$ which "violates optimality the most." Perform a line search in the direction from \mathbf{x}_k towards that point. Repeat until convergence
- ▶ Names: Frank–Wolfe, Simplicial decomposition. Chapter 12

 $\mathbf{x}^* \in \mathcal{S}$ is stationary iff

$$\mathbf{x}^* = \operatorname{Proj}_{\mathcal{S}}[\mathbf{x}^* - \nabla f(\mathbf{x}^*)]$$

- Proof.
- ▶ In other words, x* is stationary if and only if a step in the direction of the steepest descent direction followed by a Euclidean projection onto S means that we have not moved at all. (If not, then we obtain a descent direction towards that projected point—basis for the projection method in Chapter 12)

▶ The condition $\mathbf{x}^* = \operatorname{Proj}_S(\mathbf{x}^* - \nabla f(\mathbf{x}^*))$ holds if the angle between $-\nabla f(\mathbf{x}^*)$ and any feasible direction is at least 90° . These 'outwards' directions is called the **normal cone** at \mathbf{x}^* , denoted $N_S(\mathbf{x}^*)$.

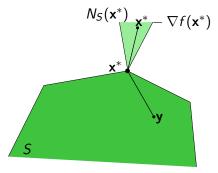


Figure: Normal cone characterization of a stationary point

Necessary optimality conditions, IV: Normal cone, 2 **Optimality**

▶ More formally, suppose $S \subseteq \mathbb{R}^n$ is closed and convex. Let $\mathbf{x} \in \mathbb{R}^n$. Then, the **normal cone** to S at \mathbf{x} is the set

$$\mathcal{N}_{\mathcal{S}}(\mathbf{x}) := egin{cases} \{ \, \mathbf{v} \in \mathbb{R}^n \mid \mathbf{v}^{\mathrm{T}}(\mathbf{y} - \mathbf{x}) \leq 0, & \mathbf{y} \in \mathcal{S} \, \}, & ext{if } \mathbf{x} \in \mathcal{S}, \ \emptyset & ext{otherwise} \end{cases}$$

Characterization of stationary point at $\mathbf{x}^* \in S$, number IV:

$$-\nabla f(\mathbf{x}^*) \in N_{\mathcal{S}}(\mathbf{x}^*) \tag{3}$$

- ▶ Equivalent to $\mathbf{x}^* = \text{Proj}_S(\mathbf{x}^*)$.
- ▶ If S is a subspace $\Longrightarrow \nabla f(\mathbf{x}^*)$ is a normal to the subspace!
- Note: if \mathbf{x}^* interior point $\Longrightarrow N_S(\mathbf{x}^*) = \{\mathbf{0}^n\}$ $(S = \mathbb{R}^n \Longrightarrow \nabla f(\mathbf{x}^*) = \mathbf{0}^n)$
- Condition IV is the only version of the necessary conditions for convex sets that extends to non-convex sets (will be

- $ightharpoonup x^*$ local min on closed convex set $S \Longrightarrow x^*$ stationary
- ▶ \mathbf{x}^* stationary AND problem convex $\Longrightarrow \mathbf{x}^*$ global min on S
- $\triangleright S = \mathbb{R}^n$: $\nabla f(\mathbf{x}^*) = \mathbf{0}^n$
- Four equivalent stationarity conditions for convex sets S:

1.
$$S \subset \mathbb{R}^n$$
: (I) VI: $\nabla f(\mathbf{x}^*)^{\mathrm{T}}(\mathbf{x} - \mathbf{x}^*) \geq 0$ for all $\mathbf{x} \in S$

2.
$$S \subset \mathbb{R}^n$$
: (II) Projection: $\mathbf{x}^* = \text{Proj}_{S}[\mathbf{x}^* - \nabla f(\mathbf{x}^*)]$

3.
$$S \subset \mathbb{R}^n$$
: (III) LP: $\min_{\mathbf{y} \in S} \nabla f(\mathbf{x}^*)^{\mathrm{T}}(\mathbf{y} - \mathbf{x}^*) = 0$

4.
$$S \subset \mathbb{R}^n$$
: (IV) Normal cone: $-\nabla f(\mathbf{x}^*) \in N_S(\mathbf{x}^*)$

Only (IV) can be extended to the case of non-convex sets S (the Karush-Kuhn-Tucker [KKT] conditions, Lecture 5−6)